Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First Principles Prediction of Topological Phases in Thin Films of Pyrochlore Iridates[1] XIANG HU, The University of Texas at Austin, ZHICHENG ZHONG, Vienna University of Technology, GREGORY A. FIETE, The University of Texas at Austin — We make materials-specific predictions for topological phases using density functional theory combined with Hartree-Fock theory that includes the full orbital structure of the relevant iridum d-orbitals and the strong but finite spin-orbit coupling strength. We find $Y_2Ir_2O_7$ bilayer and trilayer films grown along the [111] direction can respectively support a Z_2 topological metallic phase and a Chern metallic phase with a direct gap of up to 0.02 eV. These results could potentially bring transition metal oxides to the fore as a new class of topological materials with potential applications in oxide electronics.

[1]Funded by ARO Grant No. W911NF-09-10527, NSF Grant No. DMR-0955778, and DARPA grant No. D13AP00052. TACC provides computational resources.

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Date submitted: 14 Nov 2014 Electronic form version 1.4